TEXAS RESEARCHERS PIVOT TO COVID-19

TACCSTER symposium features scholars who refocused on the 2020 pandemic

Published on September 25, 2020 by Aaron Dubrow

TACCSTER 2020 was held virtually on September 17-18, 2020. It drew a larger attendance than ever before and showcased research from across Texas.

If you were looking for a snapshot of the variety of computational science research today, and its widespread impact, you couldn't find a better example than the 2020 TACC Symposium for Texas Researchers (TACCSTER) (https://www.tacc.utexas.edu/taccster) meeting.

The 270 computational scientists, engineers, scholars, and students from across Texas who gathered virtually in September 2020 were treated to presentations spanning black hole physics, environmental biology, neuroscience, quantum computing, and more.

Now in its third year, the symposium continued to grow despite a turn to remote communication facilitated by Zoom and Slack. The two keynote talks, eight research presentations, and 12 lightning talks were streamed live on Zoom, while each of the 23 posters had its own Slack channel for presentation and discussion. Three tutorials on advanced computing techniques rounded out the offerings.

This year's conference had a focus on COVID-19, including among researchers who were working on very different problems only a year ago.

Kiran Bhaganagar (https://www.tacc.utexas.edu/taccster-2020/speaker-bios#bhaganagar), associate professor of Mechanical Engineering at The University of Texas at San Antonio, had previously applied her knowledge of turbulence and atmospheric science to rapid simulations of chemical weapons attacks. But when it became clear

that COVID-19 was most frequently transmitted through droplets in the air, what was a biological problem became – at least in part – an atmospheric science one.

In her talk at TACCSTER, she described this evolution and the ways TACC supercomputers helped advance her work.

"The interdisciplinary TACCSTER conference is a valuable platform to introduce students to the wide spectrum of computational work in various disciplines from very small nano-scales to very large geophysical scales," Bhaganagar said.

Suman Sirimulla (https://www.tacc.utexas.edu/taccster-2020/speaker-bios#sirimulla), an assistant professor of Medicinal Chemistry at UT El Paso, discussed his role in the COVID-19 Drug Discovery Consortium (http://covid19ddc.com/), a group that leveraged TACC clusters to screen billions of molecules against coronavirus starting in March.

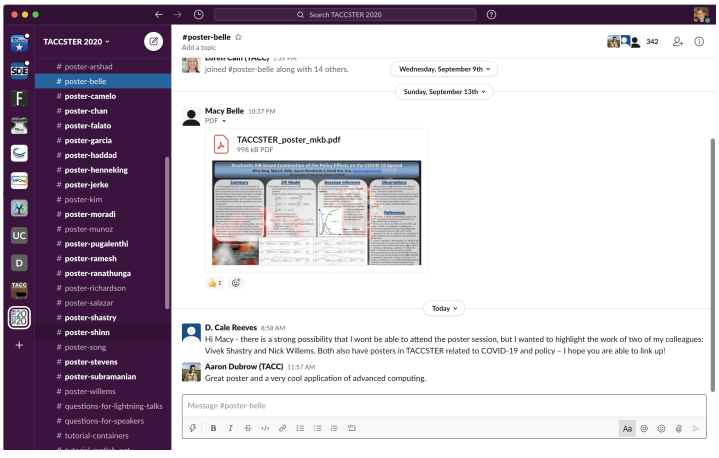
Because of his position at a UT System institution, Sirimulla was able to ramp up his research quickly to use existing pipelines and workflows on TACC supercomputers to find target compounds that might lead to treatments for COVID-19.

"The studies we're trying to do are not feasible on small compute clusters," Sirimulla said. "Screening millions of compounds against many proteins — that's a lot of computation and we wanted to get this done in a few days. So we needed clusters like TACC's."

Lauren Ancel Meyers (https://www.tacc.utexas.edu/taccster-2020/speaker-bios#meyers), the keynote speaker and Cooley Professor of Integrative Biology and Statistics & Data Science at UT Austin, described how she and her team developed one of the leading epidemiological models of the COVID-19 pandemic.

The model, built in collaboration with TACC experts and other UT Austin researchers, has been used by local, state, and national leaders to inform decisions about when to institute lockdowns and open schools.

"All of this work is only possible because of our collaboration — not just now, but over the past two decades — with TACC in everything we do," Meyers said. "The people at TACC have been true partners in helping us to envision what it is we want to do, to make it happen, and to provide all the resources we could possibly need to do the large computational work we do."



A screenshot of the TACCSTER 2020 slack channel showing poster session conversations in progress.

In his lightning talk, Vivek Shastry, a doctoral student at UT Austin's LBJ School of Public Affairs, introduced the COVID-19 Policy Evaluation (COPE) tool developed by his team. Using the tool, Shastry simulated realistic shelter-in-place policy designs and behavioral response scenarios.

"So far, the key finding has been the relatively strong influence of timing of shelter-in-place orders in reducing hospitalization from COVID-19," Shastry explained in the Slack poster session

Nick Willems, a PhD student in Mechanical Engineering at UT Austin presented related work on an agent-based model of the social spread of COVID-19 that incorporates heterogeneity in populations and behaviors — for example, risk-taking.

"We simulated individual interactions to arrive at emergent macro-level disease progressions," Willems explained.

Two researchers described efforts that touch on the societal effects of the pandemic. Assistant Professor of Economic, Political and Policy Sciences at UT Dallas Rebecca Cordell (https://www.tacc.utexas.edu/taccster-2020/speaker-bios#cordell) discussed the results of her research on the relationship between social unrest and pandemics. She realized her study of disease outbreaks and unrest in Africa between 1991-2006 could be educational for COVID-19.

"We knew the research was current and that we needed to get it out there," Cordell said. "TACC came to the rescue."

Cordell's application for compute time on TACC systems was fast-tracked because of its relationship to COVID-19.

"We were able to run models in XSEDE" — the Extreme Science and Engineering Discovery environment of which TACC is a part — "specifically Jetstream. It's easy to use and maintain and provides great storage."

In his invited talk, Matt Lease (https://www.tacc.utexas.edu/taccster-2020/speaker-bios#lease), associate professor in the School of Information at UT Austin, demonstrated a new tool (https://exfacto.herokuapp.com/) his team is developing to help citizens fact-check claims. The tool provides not only a True/False assessment, but presents the data (in the form of links to web articles), and the confidence in the assessment for the viewer to see.

In addition to a "veracity" measure, his tool includes a separate user-based "reliability" measure that helps users both accept findings and identify their own biases. The tool has the potential to prevent the spread of misinformation and even change minds about entrenched ideas. This is especially important given the negative effects of misinformation during the pandemic.

The pivot to COVID-19 research isn't limited to researchers. As an organization, TACC changed its policies and focus to address the pandemic, explained TACC Executive Director Dan Stanzione.

"About 30 percent of the time on Frontera has been diverted to emergency COVID response work since March," Stanzione shared.

This includes not only Meyers' epidemiological modeling and Sirimulla's small molecule docking research, but AI-driven drug discovery research by Department of Energy Researchers; molecular modeling of the spike protein by UC San Diego researchers; genomic analyses to better understand the evolution of the virus by the Galaxy bioinformatics community; and 50 other COVID-19 projects, more than 20 of them led by Texas researchers.

"Making the best of a bad situation, we've shown how computing can be used in these times of national crisis to do good things that hopefully show benefits in the not-so-distance future, and in some cases are showing benefits already," Stanzione concluded.

NEWS CATEGORIES

User News (https://portal.tacc.utexas.edu/user-news)
Press Releases (https://www.tacc.utexas.edu/news/press-releases)
Feature Stories (https://www.tacc.utexas.edu/news/feature-stories)